LA-UR-17-25633
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Title: The Monte Carlo Method and MCNP - A Brief Review of Our 40 Year History

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Intended for: IRRMA X, 2017-07-09 (Chicago, Illinois, United States)

Issued: 2017-07-11

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# The Monte Carlo Method and MCNP – A Brief Review of Our 40 Year History

## Presentation to the International Topical Meeting on Industrial Radiation and Radioisotope Measurement Applications Conference

**Avneet Sood, PhD**

**XCP-3 Group Leader**

10 July 2017

Los Alamos NATIONAL LABORATORY EST.1943



**LA-UR-17-XXXX**

# Outline

- **Origins of the Monte Carlo method**
  - Development of electronic computers and Monte Carlo method occur simultaneously
  - Ulam, Von Neumann, Richtmeyer, Metropolis, Fermi
- **Growth and usage of Monte Carlo codes**
  - 1950's, 1960's, and 1970's
    - Monte Carlo becomes mainstream; nuclear criticality and reactor
- **Emergence of MCNP**
- **MCNP's history**
- **MCNP's upcoming future**

***nearly all references can be found at: https://laws.lanl.gov/vhosts/mcnp.lanl.gov/references.shtml**

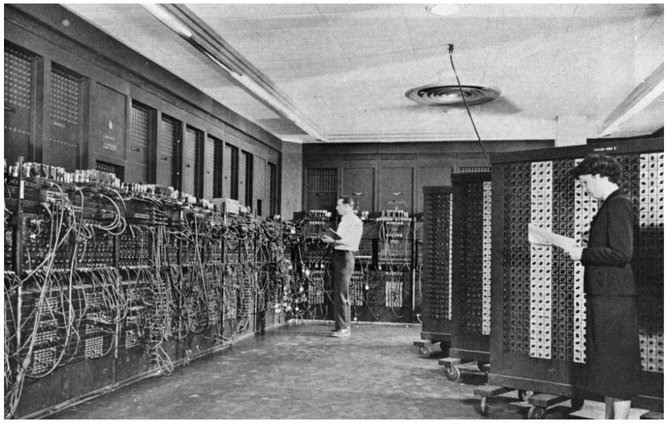
# Abstract

The Monte Carlo method for radiation particle transport has its origins at LANL dating back to the 1940's. The creators of these methods were Drs. Stanislaw Ulam, John von Neumann, Robert Richtmyer, and Nicholas Metropolis. Monte Carlo methods for particle transport have been driving computational developments since the beginning of modern computers; this continues today. In the 1950's and 1960's, these new methods were organized into a series of special-purpose Monte Carlo codes, including MCS, MCN, MCP, and MCG. These codes were able to transport neutrons and photons for specialized LANL applications. In 1977, these separate codes were combined to create the first generalized Monte Carlo radiation particle transport code, MCNP. In 1983, MCNP3 was released for public distribution to the Radiation Safety Information Computational Center (RSICC). The upcoming release of MCNP (version 6.2) is expected in June 2017. Approximately 20,000 copies of MCNP have been distributed to users in government institutions, academia, and private industries worldwide. This talk will review our history, current status, and future directions.

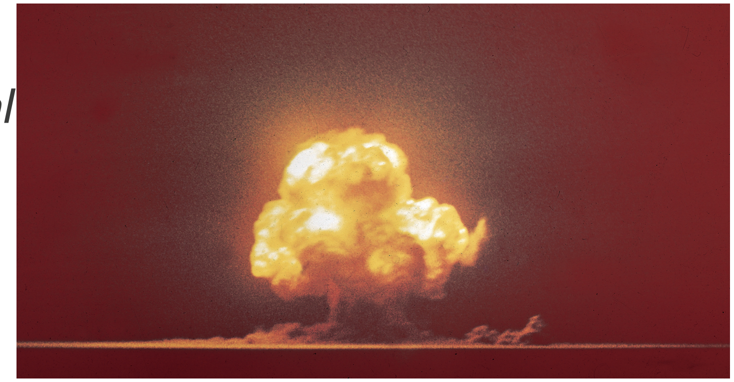
# The Origins of Monte Carlo – 1946 Stanislaw Ulam

- “*The year was 1945. Two earthshaking events took place: the successful test at Alamogordo and the building of the first electronic computer*” – N. Metropolis
- **The method was invented by Stanislaw Ulam in 1946 playing Solitaire while recovering from an illness.**
- “*After spending a lot of time trying to estimate success by combinatorial calculations, I wondered whether a more practical method…might be to lay it out say one hundred times and simply observe and count the number of successful plays*” – S. Ulam

Stanislaw Ulam



ENIAC– the first electronic computer, University of Pennsylvania. Solved ballistic trajectory problems for Army Ballistics Research Lab. Used electron tubes instead of mechanical counters. Minutes instead of days. Declassified in 1946.



Trinity – code name for first nuclear detonation

“Stan Ulam, John von Neumann, and the Monte Carlo Method,” R. Eckhardt, Los Alamos Science Special Issue 1987.

# The Origins of the Monte Carlo Method

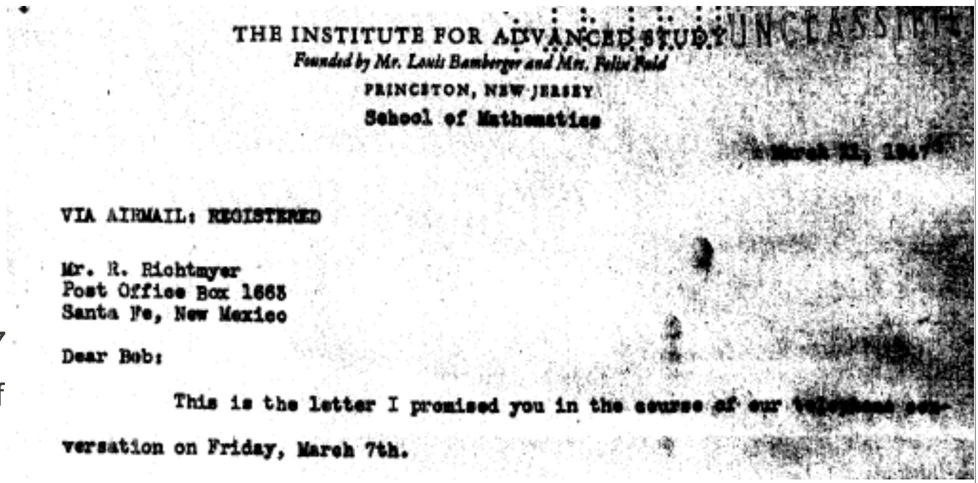
- **Ulam describes this idea to John von Neumann in a conversation in 1946**
- **Von Neumann is intrigued**
  - 1943: Electro-Mechanical computers solved non-linear diff. eq. via production line. Punch card used for every point in space/time
  - New computers could count/arithmetic and hence solve difference equations (BRL at Aberdeen, MD)
  - Statistical sampling on electronic computers
  - Especially suitable for exploring neutron chain reactions in fission – neutron multiplication rates
- **R.D Richtmyer and J. von Neumann "Statistical Methods in Neutron Diffusion", Los Alamos (LAMS-557) April 9, 1947.**
  - Detailed letter from John von Neumann to Robert Richtmyer describing a conversation in March 1947
    - "I have been thinking a good deal about the possibility of using statistical methods to solve neutron diffusion and multiplication problems in accordance with the principle suggested by Stan Ulam"
    - Letter contained 81-step pseudo code for using MC for particle transport

John von Neumann

J. Von Neumann invented scientific computing in the 1940's

- Stored programs now called software
- Algorithms/Flowcharts
- Hardware design

Consultant to Aberdeen and Los Alamos



THE INSTITUTE FOR ADVANCED STUDY
*Founded by Mr. Louis Bamberger and Mrs. Felix Fuld*
PRINCETON, NEW JERSEY
School of Mathematics

March 11, 1947

VIA AIRMAIL: REGISTERED

Mr. R. Richtmyer
Post Office Box 1663
Santa Fe, New Mexico

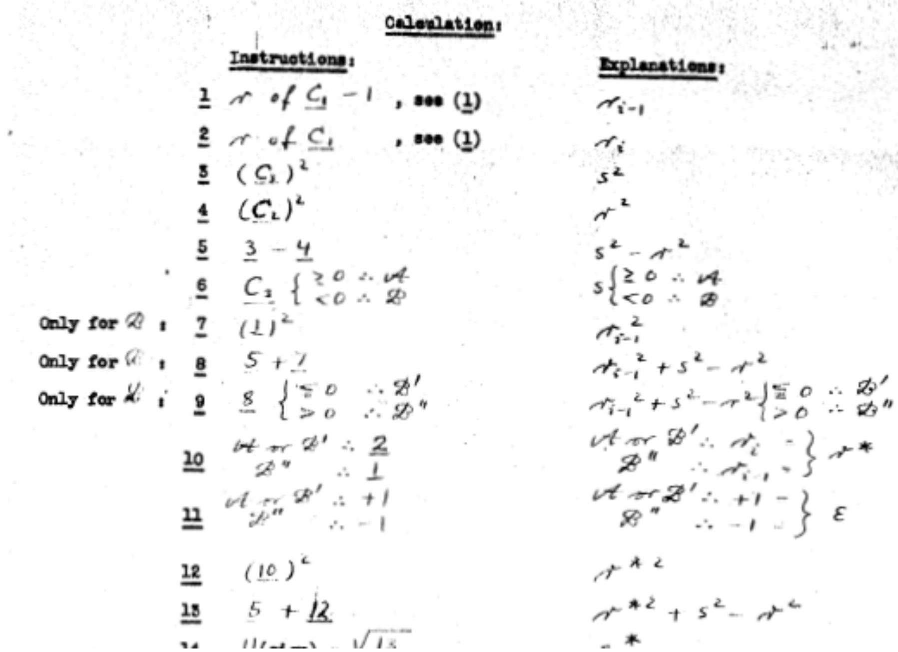
Dear Bob:

This is the letter I promised you in the course of our telephone conversation on Friday, March 7th.

# The first Monte Carlo (pseudo) Code - 1947

- **Von Neumann's Assumptions:**
  - Time-dependent, continuous energy, spherical but radially-varying, 1 fissionable material, isotropic scattering and fission production, fission multiplicities of 2,3, or 4
- **Suggested 100 neutrons each to be run for 100 collisions**
  - Thought these were too much
- **Estimated time: 5 hrs on ENIAC**
- **Richtmyer's response:**
  - Very interested in idea and proposed suggestions
    - Allow for multiple fissionable materials, no fission spectrum energy dependence, single neutron multiplicity, run for computer time not collisions
- **ENIAC: first calculations run April/May 1948**
  - Code finalized in **December 1947**;
  - Continuous energy neutrons, fission spectra and XS tabulated at interval mid-points, histogram energy-dependence of XS, pseudo-RN.

Thomas Haight, et al., "Los Alamos Bets on ENIAC: Nuclear Monte Carlo Simulations, 1947-1948, IEEE Ann. Of History of Comp July-Sept 2014



**Calculation:**

| | | Instructions: | Explanations: |
|---|---|---|---|
| | 1 | $r$ of $C_1 - 1$, see (1) | $r_{i-1}$ |
| | 2 | $r$ of $C_1$, see (1) | $r_i$ |
| | 3 | $(C_1)^2$ | $s^2$ |
| | 4 | $(C_2)^2$ | $r^2$ |
| | 5 | $3 - 4$ | $s^2 - r^2$ |
| | 6 | $C_3 \begin{cases} \geq 0 \therefore \mathcal{A} \\ < 0 \therefore \mathcal{B} \end{cases}$ | $s \begin{cases} \geq 0 \therefore \mathcal{A} \\ < 0 \therefore \mathcal{B} \end{cases}$ |
| Only for $\mathcal{B}$: | 7 | $(1)^2$ | $r_{i-1}^2$ |
| Only for $\mathcal{B}$: | 8 | $5 + 7$ | $r_{i-1}^2 + s^2 - r^2$ |
| Only for $\mathcal{B}$: | 9 | $8 \begin{cases} \leq 0 \therefore \mathcal{B}' \\ > 0 \therefore \mathcal{B}'' \end{cases}$ | $r_{i-1}^2 + s^2 - r^2 \begin{cases} \leq 0 \therefore \mathcal{B}' \\ > 0 \therefore \mathcal{B}'' \end{cases}$ |
| | 10 | $\mathcal{A}$ or $\mathcal{B}' \therefore 2$; $\mathcal{B}'' \therefore 1$ | $\left.\begin{matrix} \mathcal{A} \text{ or } \mathcal{B}' \therefore r_i \\ \mathcal{B}'' \therefore r_{i-1} \end{matrix}\right\} r^*$ |
| | 11 | $\mathcal{A}$ or $\mathcal{B}' \therefore +1$; $\mathcal{B}'' \therefore -1$ | $\left.\begin{matrix} \mathcal{A} \text{ or } \mathcal{B}' \therefore +1 \\ \mathcal{B}'' \therefore -1 \end{matrix}\right\} \varepsilon$ |
| | 12 | $(10)^2$ | $r^{*2}$ |
| | 13 | $5 + 12$ | $r^{*2} + s^2 - r^2$ |

R.D Richtmyer and J. von Neumann "Statistical Methods in Neutron Diffusion", Los Alamos (LAMS-557) April 9, 1947.

April 2, 1947

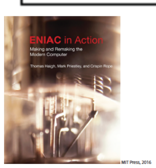
Professor John vonNeumann,
The Institute for Advanced Study,
School of Mathematics
Princeton, New Jersey

Dear Johnny:

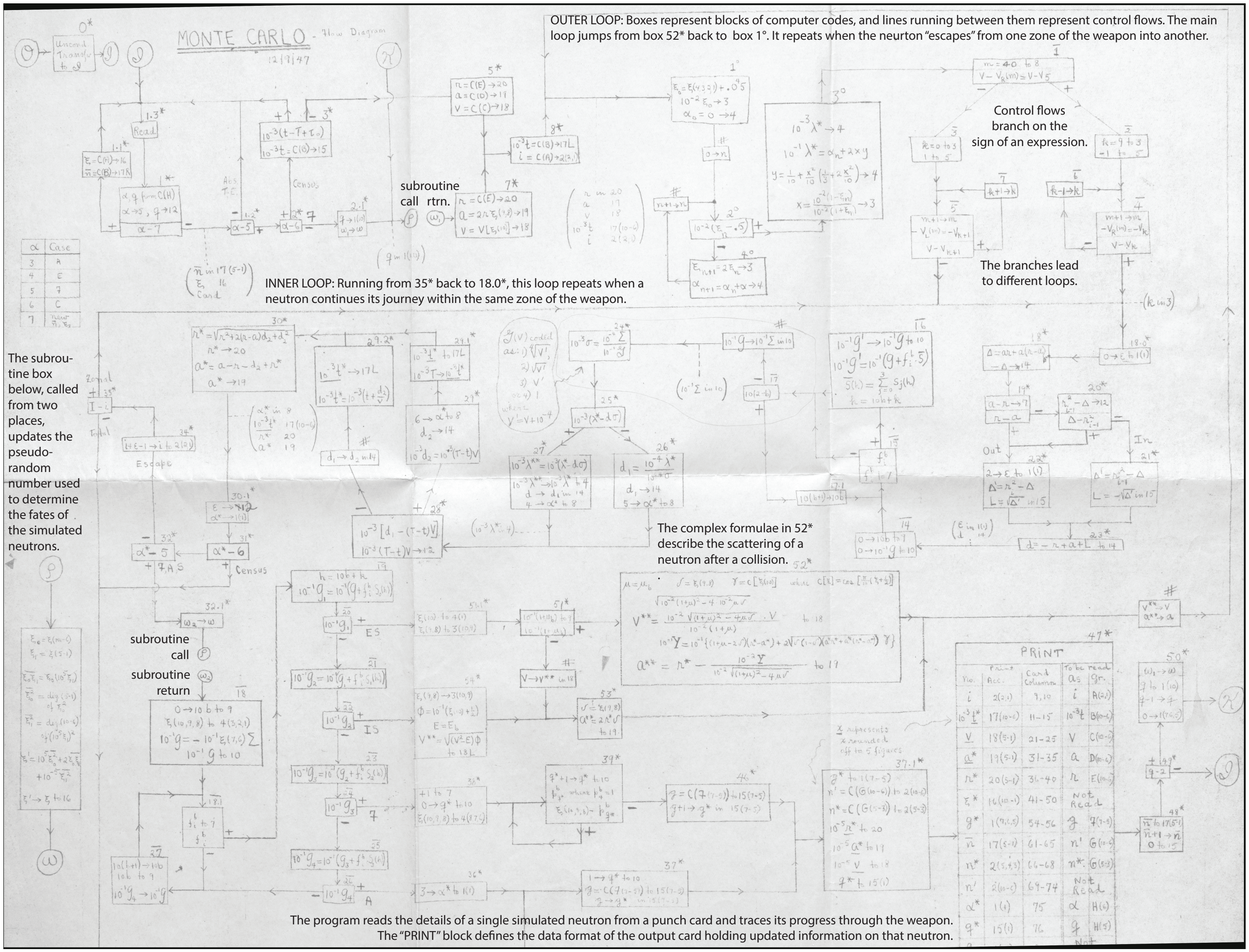
As Stan told you, your letter has aroused a great deal of interest here. We have had a number of discussions of your method and Bengt Carlson has even set to work to test it out by hand calculation in a simple case.

# ENIAC in Action:

| Boxes | Function |
|---|---|
| 1* – 8* | Read a card and store neutron characteristics |
| 1° – 4° | Calculate random parameter λ* |
| $\overline{1}$ – $\overline{7}$ | Find neutron's velocity interval |
| 18* – 23* | Calculate distance to zone boundary |
| $\overline{14}$ – $\overline{17.1}$, 24* | Calculate cross-section of material in zone |
| 25* – 27* | Determine if terminal event is collision or escape |
| 28* – 30* | Determine if a census comes first |
| 31* – 35* | Discriminate between terminal events |
| Subroutine p/ω | Refresh random number |
| $\overline{18}$ – $\overline{27}$ | Determine collision type |
| 51* – 52* | Elastic scattering |
| 53* – 54* | Inelastic scattering |
| 36* – 39*, 46* | Absorption/fission |
| 37.1*, 47* – 50* | Print card and restart main loop |

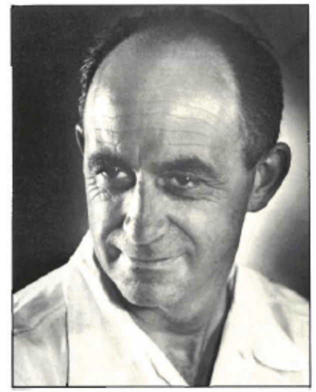


Thomas Haight, Mark Priestley, and Crispin Rope, "ENIAC in Action: Making and Remaking the Modern Computer," MIT Press 2016

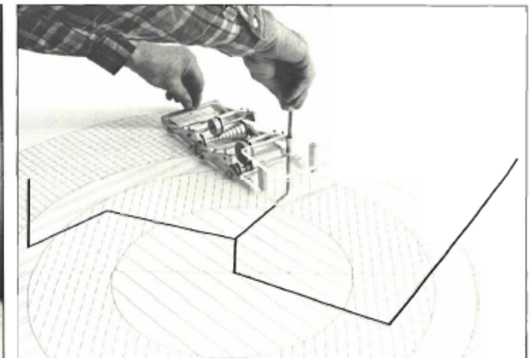


# Enrico Fermi: Independently developed Monte Carlo!

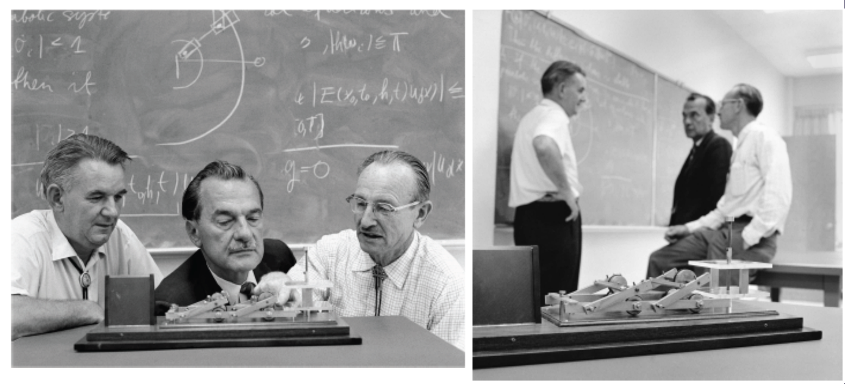
- **Emilio Segre, Fermi's student and collaborator:**
  - *"Fermi had invented, but of course not named, the present Monte Carlo method when he was studying the moderation of neutrons in Rome. He did not publish anything on the subject, but he used the method to solve many problems with whatever calculating facilities he had, chiefly a small mechanical adding machine"*
- **Astonished Roman colleagues when he would predict experimental results remarkably accurately. He revealed that he used statistical sampling techniques whenever insomnia struck.**
- **15 years prior to Ulam**
- **While in Los Alamos and awaiting ENIAC's move, he created an analog device to study neutron transport.**
  - Called FERMIAC
  - Generated the site of next collision based upon characteristics of material; Another choice was made at boundary crossing; "slow" and "fast" neutron energies



Enrico Fermi



FERMIAC



Los Alamos Scientists: Bengt Carlson, Nicholas Metropolis, LDP King with Fermiac (1966)

# MANIAC – Nicholas Metropolis

- **Post-war ENIAC started a revolution that continues today**
- **MANIAC – Mathematical and Numerical Integrator and Computer**
  - Was a product of Nicholas Metropolis at LANL; borrowed concepts from von Neumann's IAS, operational in 1952;
  - MADCAP – high-level language and compiler
  - Rapid growth of computing: AVIDAC (Argonne) ORACLE (Oak Ridge), ILLIAC (U of I)
  - Special effort that helped bind Von Neumann, Fermi, Beta, Teller, Ulam, Feynman, etc in post-war efforts. MANIAC was a fascination.
  - First time "Monte Carlo" appears in publication:
    - Nicholas Metropolis and S. Ulam , "The Monte Carlo Method," *Journal of the American Statistical Association* Vol. 44, No. 247 (Sep., 1949)
  - MC on MANIAC used for multiple problems other than radiation transport:

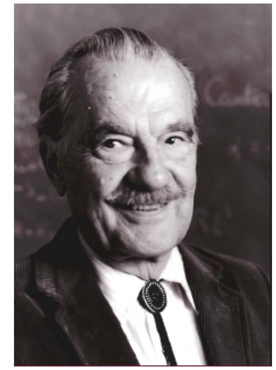
JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION

*Number 247* SEPTEMBER 1949 *Volume 44*

THE MONTE CARLO METHOD

NICHOLAS METROPOLIS AND S. ULAM
*Los Alamos Laboratory*

We shall present here the motivation and a general description of a method dealing with a class of problems in mathematical physics. The method is, essentially, a statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of the natural sciences.



Pion-proton phase-shift analysis (Fermi, Metropolis; 1952)
Phase-shift analysis (Bethe, deHoffman, Metropolis; 1954)
Nonlinear coupled oscillators (Fermi, Pasta, Ulam; 1953)
Genetic code (Gamow, Metropolis; 1954)
Equation of state: Importance sampling (Metropolis, Teller; 1953)
Two-dimensional hydrodynamics (Metropolis, von Neumann; 1954)
Universalities of iterative functions (Metropolis, Stein, Stein; 1973)
Nuclear cascades using Monte Carlo (Metropolis, Turkevich; 1954)
Anti-clerical chess (Wells; 1956)
The lucky numbers (Metropolis, Ulam; 1956)

# 1950's: Monte Carlo is becoming mainstream!

- **Herman Kahn, "Applications of Monte Carlo," AECU-3259 (April 19, 1954).**
  - General and not specific to radiation particle transport
  - Direct sampling for common distributions
  - Rejection sampling – if direct sampling does not work
    - Use a simple, easy to sample distribution, to get an estimate and correct later.
  - Russian Roulette
  - Stratified sampling, importance sampling, splitting
- **E.D. Cashwell and C.J. Everett, "A Practical Manual on the Monte Carlo Method for Random Walk Problems," LA-2120 (December 18, 1957)**
  - Well-described report specific to particle transport
  - Detailed diagrams and flowcharts
    - Neutron collisions – (in)elastic scattering, fission, etc
    - Photon collisions – Compton scattering, photoelectric, pair prouction
    - Particle direction after collision – direction cosines
  - Did not deal with thermal neutron collisions nor pseudo-random number generation

Thomas Sutton and David Griesheimer, "The Monte Carlo Method: The Past 70 Years, Current State and Future Prospects," ANS Math and Computational Division Topical (Jeju, South Korea, April 2017)

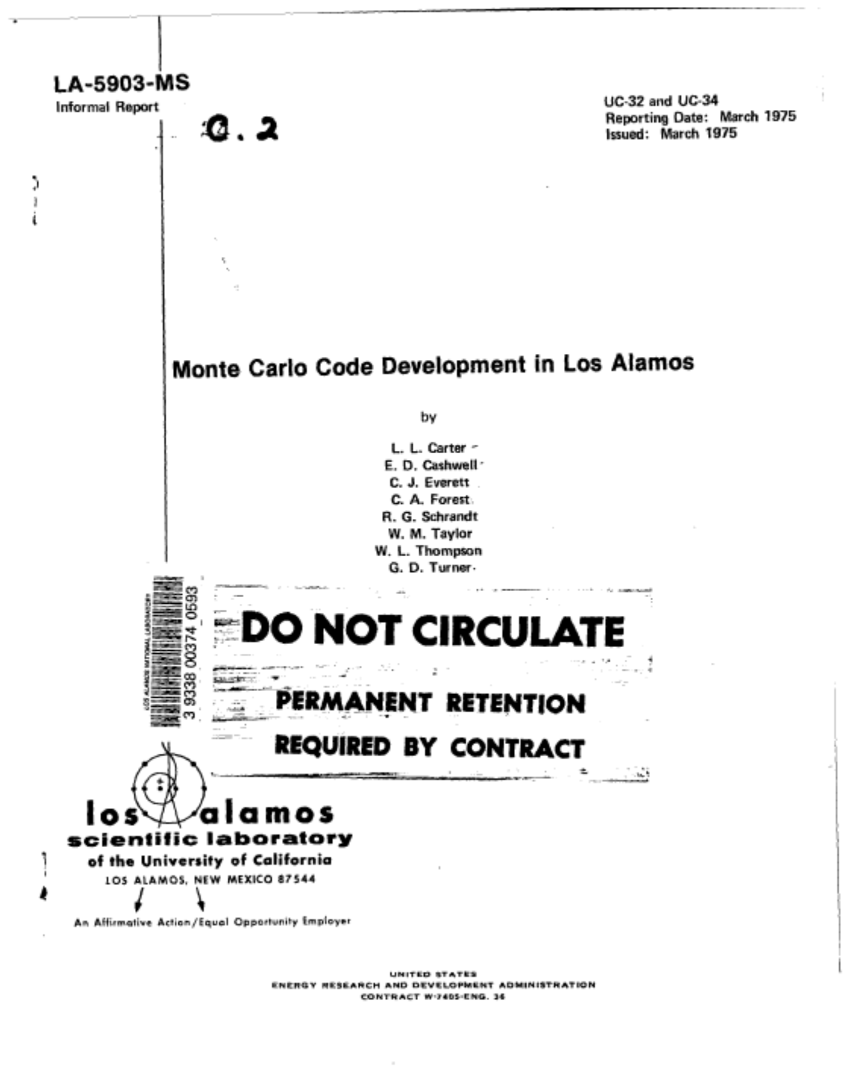
# 1960's: Initial work on Criticality and Reactor Calculations

- **JJ.B. Parker, and E.R. Woodcock, "Monte Carlo Criticality Calculations," Prog. In Nucl. Ener, 4 (1961).**
  - Introduced concept of neutron generations or batches of particles as histories
- **E.R. Woodcock, T. Murphy, P.J. Hemmings, and T.C. Longworth, "Techniques Used in the GEM Code for Monte Carlo Neutronics Calculations in Reactors and Other Systems of Complex Geometry," ANL-1050 (1965).**
  - Describes "Woodcock tracking" (aka delta-tracking)
    - Regular tracking on geometries with many surfaces is expensive; esp for 2nd order surfaces
    - Avoids multiple distance-to-boundary calculations by using fictitious XS and adjusting
- **J. Lieberoth, "A Monte Carlo Technique to Solve the Static Eigenvalue Problem of the Boltzmann Transport Equation," Nukleonik 11, 213-219 (1968)**
- **M.R. Mendelson, "Monte Carlo Criticality Calculations for Thermal Reactors," Nucl. Sci. Eng 32, 319-331 (1968).**

Thomas Sutton and David Griesheimer, "The Monte Carlo Method: The Past 70 Years, Current State and Future Prospects," ANS Math and Computational Division Topical (Jeju, South Korea, April 2017)

# 1970: MCNP first emerges

- **1974 – NEA Committee on Reactor Physics (NEACRP)**
  - E.D. Cashwell presented a paper on Monte Carlo development at Los Alamos
    - MCN – neutrons
    - MCNA – neutron adjoint
    - MCG – gamma rays
    - MCP – general photons
    - MCNG – coupled neutron-gamma ray
    - MCMG – multi-group coupled neutron-gamma ray
    - MCGE – coupled electron-photon
    - MCGB – gamma rays with Bremsstrahlung
- **1977: MCNG was merged with MCP to form MCNP**
  - 2017 is the 40th Anniversary of MCNP
  - 2017 is also the 70th Anniversary of the Monte Carlo method



LA-5903-MS
Informal Report

C. 2

UC-32 and UC-34
Reporting Date: March 1975
Issued: March 1975

Monte Carlo Code Development in Los Alamos

by

L. L. Carter
E. D. Cashwell
C. J. Everett
C. A. Forest
R. G. Schrandt
W. M. Taylor
W. L. Thompson
G. D. Turner

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CONTRACT W-7405-ENG. 36

# Monte Carlo & MCNP History

**ENIAC – 1945**

30 tons

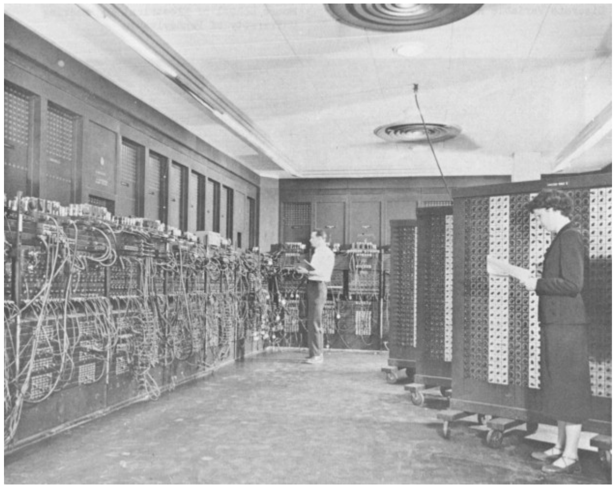
20 ft x 40 ft room

18,000 vacuum tubes

0.1 MHz

20 word memory

patchcords



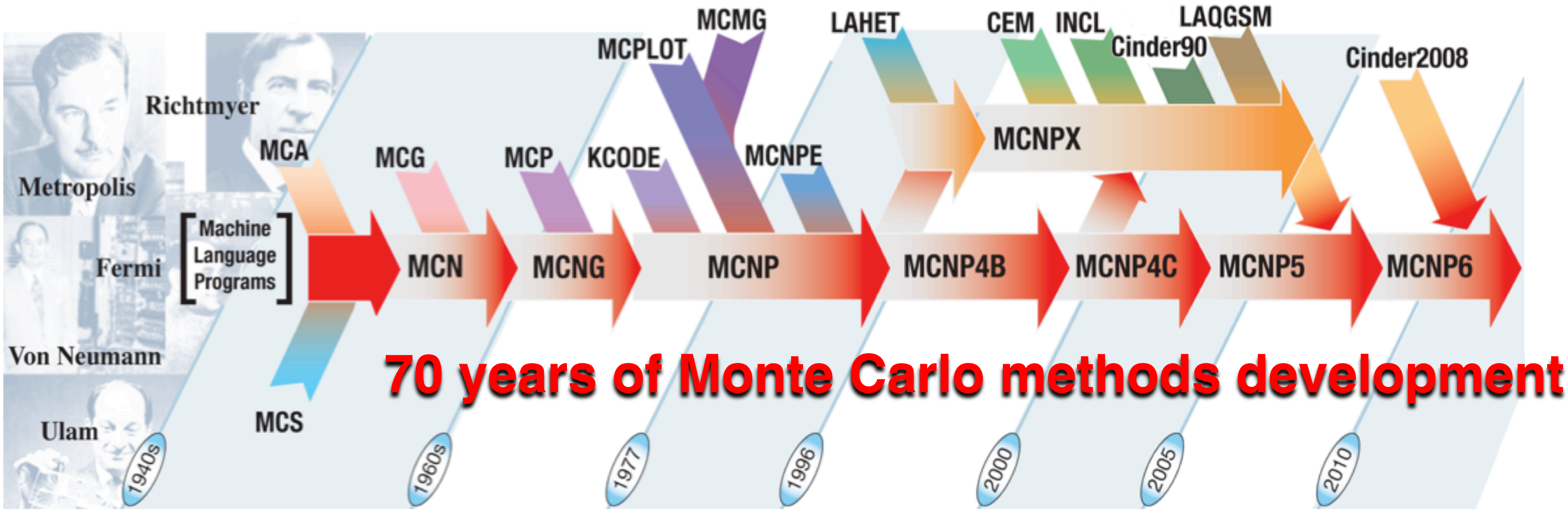
**Manhattan Project – 1945...**

Discussions on using ENIAC

**Ulam** suggested using the "method of statistical trials"

**Metropolis** suggested the name "Monte Carlo"

**Von Neumann** developed the first computer code



# 1980 – 1999: MCNP Becomes the Gold Standard

| MCNP Version | Release Month/Year | Some Significant New Features (For a more detailed description, see each version's release notes). |
|---|---|---|
| MCNP3 | 1983 | First release through RSICC. Written in Fortran 77 |
| MCNP3A | 1986 | |
| MCNP3B | 1988 | Plotting graphics, generalized source, surface sources, repeated structures/lattice geometries |
| MCNP4 | 1990 | Parallel multitasking, electron transport |
| MCNP4A | 10/1993 | Enhanced statistical analysis, new photon libraries, ENDF-6, color X-Windows graphics, dynamic memory allocation |
| MCNP4B | 4/1997 | Operator perturbations, enhanced photon physics, PVM load balancing, cross-section plotting, 64-bit executables, lattice universe mapping, enhanced lifetimes |
| MCNPX 2.1.5 | 11/1999 | First public release of MCNPX, based on MCNP4B with CEM INC, HTAPE3X, mesh and radiography tallies, and an improved collisional energy loss model. |

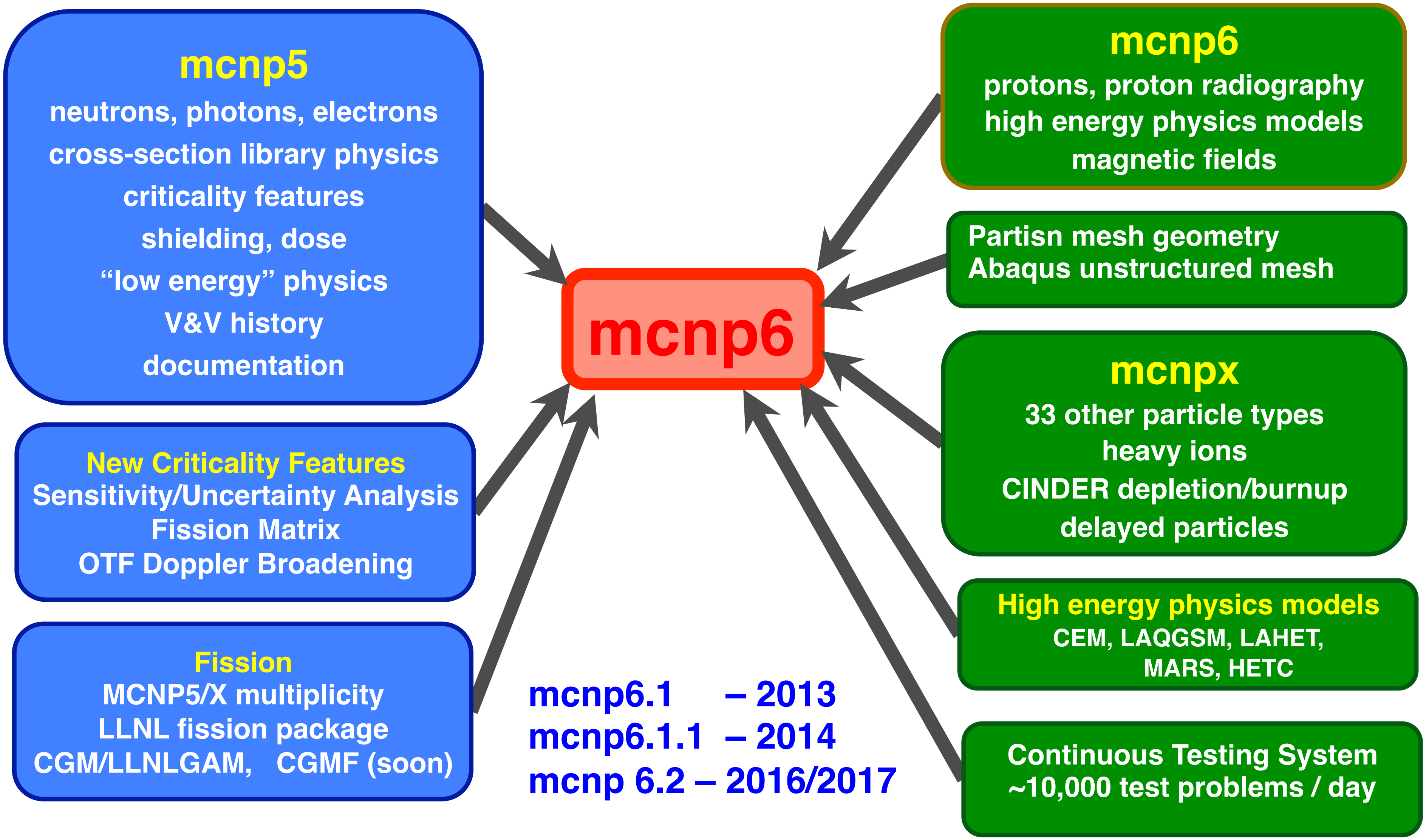
T. Goorley, et al. "Initial MCNP6 Release Overview," LA-UR-13-22934 (2013)

- **Key Value: MCNP provides a predictive capability that can replace expensive or impossible-to-perform experiments**
- **Used to design large-scale measurements providing significant time/cost savings**
- **MCNP represents a synergistic capabilities developed at LANL**
  - Evaluated nuclear data (ENDF) and data processing code NJOY
  - MCNP could not exist without this!
- **International user community's high confidence in MCNP's predictive capabilities are based upon its performance with verification and validation test suites.**

# 2000 – 2011: MCNP undergoes exponential growth

| | | |
|---|---|---|
| MCNP4C | 4/2000 | Unresolved resonance treatments, macrobodies, superimposed importance mesh, perturbation, electron transport, plotter and tally enhancements |
| MCNP4C2 | 1/2001 | Photonuclear physics, interactive plotting, plot superimposed weight-window mesh, weight-window improvements |
| MCNPX 2.3.0 | 4/ 2002 | LAHET 2.8 and some 3.0 extensions. |
| MCNPX 2.4.0 | 8/2002 | Update to MCNP4C, build system for Windows OS, support for Fortran 90. |
| MCNP5 1.14 | 11/2002 | Fortran 90, photonuclear collisions, geometry superimposed mesh tallies, time splitting, shared memory threading with OpenMP. Mac OSX support |
| MCNP5 1.20 | 10/2003 | Increased number of detectors to 100 and number of tallies to 1000. Mostly a code defect fix release. |
| MCNP5 1.30 | 8/2004 | Explicit 8-byte integers for nps > 2.1 billion, Lattice and fmesh tally enchantments. Support for MPI on Mac OSX. |
| MCNPX 2.5.0 | 4/2005 | 34 particle types, four light ions, mix and match nuclear data tables and model physics, CEM2k, INCL4/ABLA physics models, fission multiplicity, spontaneous fission sources, pulse height tallies with variance reduction, pulse height light tally, coincident capture tallies, variance reduction with model |
| MCNP5 1.40 | 11/2005 | Lethargy plots, logarithmic data interpolation, neutron multiplicity distributions, stochastic geometry, source entropy, mesh tally plots, new electron energy loss straggling |
| MCNPX 2.6.0 | 4/ 2008 | Depletion/Burnup, heavy ion transport, LAQGSM physics, CEM03 physics, delayed gamma emission, energy-time weight windows, charged ions from neutron capture, spherical mesh weight windows, spontaneous photons |
| MCNP5 1.51 | 1/2009 | Photon Doppler broadening, variance reduction with pulse height tallies, annihilation gamma tracking, Doppler broadening in makxsf, large lattice enhancements |
| MCNP5 1.60 | 8/2010 | Adjoint weighted tallies for point kinetics parameters, mesh tallies for isotopic reaction rates, up to 100 million cells & surfaces, up to 10 thousand tallies |
| MCNPX 2.7.0 | 4/2011 | Tally Tagging, embedded sources, cyclic time bins, focused beam sources, PTRAC coincidence, LLNL fission multiplicity, Receiver-operator characterization (ROC) tally, NRF data in ACE libraries, triple & quadruple coincidence, LAQGSM 3.03 and CEM 3.03 physics. |

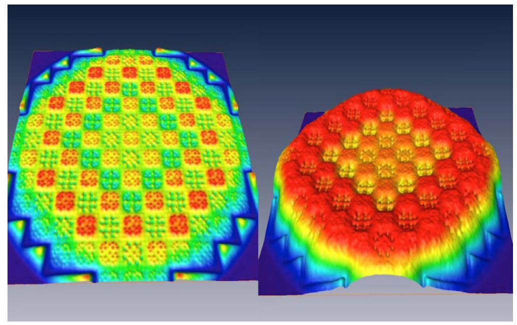
# 2011 – today:  MCNP5 & MCNPX to MCNP6

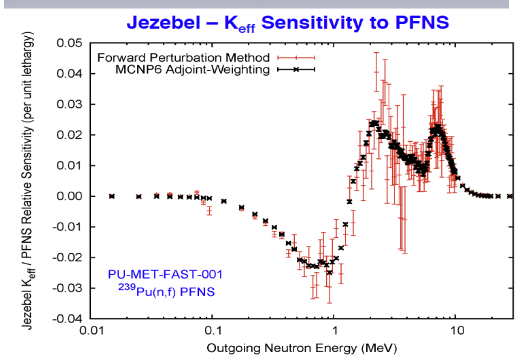


# MCNP® Capabilities

- **Physics:**
  - Continuous energy particle transport
  - Neutron, photon, electron, and many more particle types
- **Algorithms:**
  - k-eigenvalue calculations
  - Fixed source calculations
- **Recently Implemented Features:**
  - Unstructured mesh transport
  - Electric and magnetic field transport
  - High-energy physics models
  - 33 additional particle types
  - Reactor fuel depletion and burnup
  - Radiation source and detection capabilities
  - Sensitivity and uncertainty analysis for nuclear criticality safety
- **Extensive Variance Reduction**
  - Weight Windows
  - DXTRAN

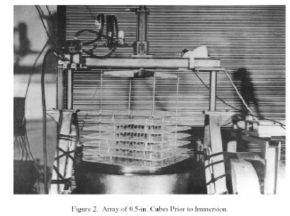
Whole-core Thermal & Total Flux



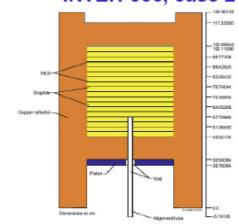


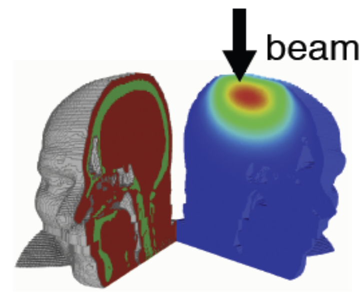

Experimental Benchmarks with Critical Assemblies

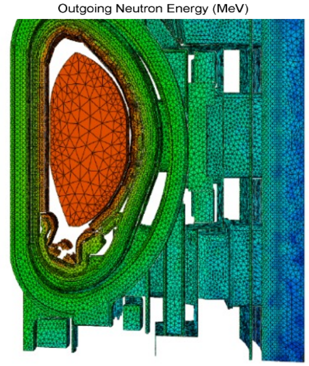
HEU-MET-THERM-003



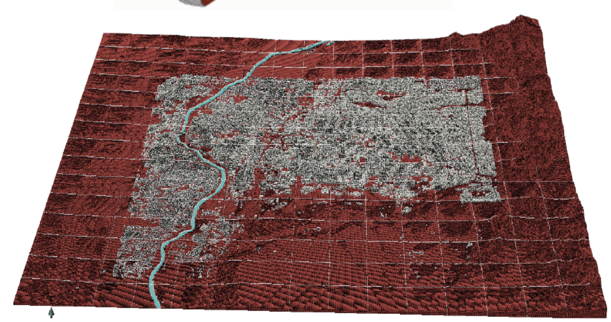
Zeus-2, HEU-MET-INTER-006, case 2





ITER Neutron Flux Calculations



City model used to study nuclear weapon effects

# Monte Carlo Codes from across the globe

- **Monte Carlo Codes Session at SNA+MC 2013**
  – Annals of Nuclear Energy, 82 (2015)

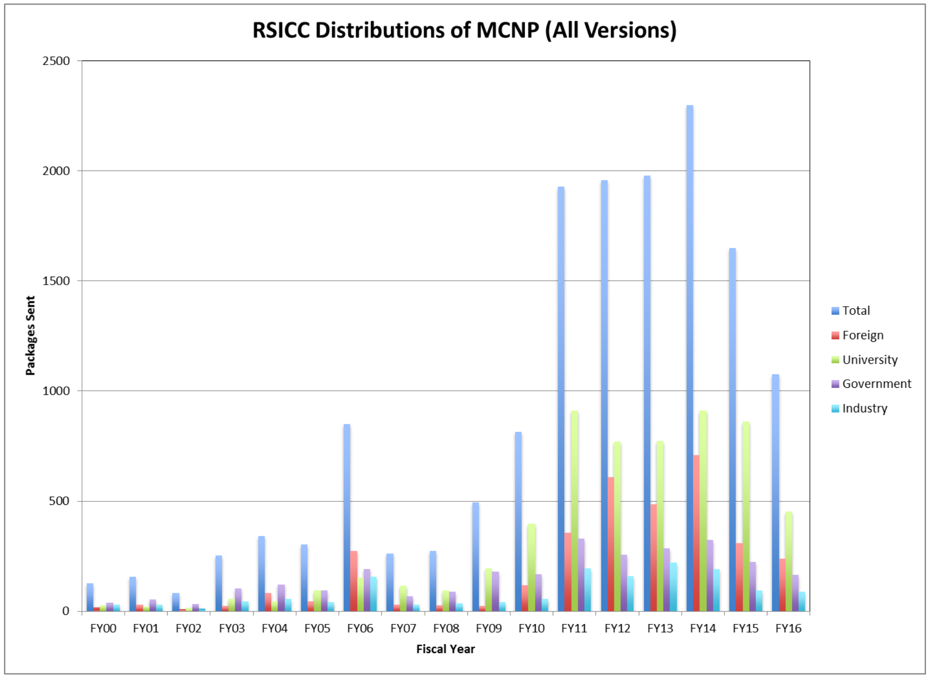
| code | institution | |
|---|---|---|
| ARCHER | RPI | USA |
| COG11 | LLNL | USA |
| DIANE | CEA | France |
| FLUKA | INFN & CERN | Italy & CERN |
| GEANT4 | GEANT4 | International |
| KENO and MONACO | ORNL | USA |
| MC21 | Naval Nucl. Lab. | USA |
| MCATK | LANL | USA |
| MCCARD | Seoul Natl. Univ. | ROK |
| MCNP6 | LANL | USA |
| MCU | Kurchatov Inst. | Russia |

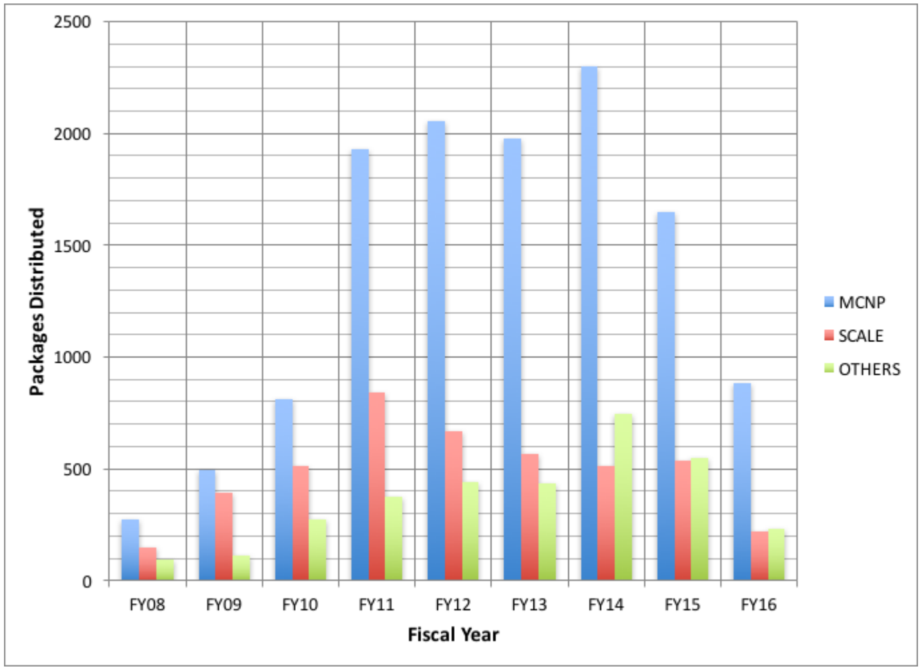
| code | institution | |
|---|---|---|
| MONK & MCBEND | AMEC Foster Wheeler | UK |
| MORET5 | IRSN | France |
| MVP2 | JAEA | Japan |
| OPENMC | MIT | USA |
| PENELOPE | Barcelona Univ. | Spain |
| PHITS | JAEA | Japan |
| PRIZMA | VNIITF | Russia |
| RMC | Tsinghua Univ. | China |
| SERPENT | VTT | Finland |
| SUPERMC | CAS INEST FDS | China |
| TRIPOLI-4 | CEA | France |

# MCNP Distribution: RSICC

- **MCNP is export controlled and is distributed:**
  - USA: RSICC – Oak Ridge National Laboratory, LANL
  - Europe: NEA Databank; Japan, Korea: KAIST – coordinated through RSICC
- **Approximately 20,000 copies of MCNP licenses have been distributed.**
  - 8000 copies of MCNP 6 since 2011 (Data provided by T. Valentine, RSICC)

**Today: All requests eventually are through RSICC or LANL with appropriate DOE / export control reviews**



# MCNP in the near future

- **Motivation: LANL, DOE/NNSA, DHS-DNDO, and DTRA sponsors need a predictive capability**
- **Biggest needs are:**
  - Validated models of geometry and materials; complex radiation sources; direct comparison with radiation detection instruments
- **MCNP 2020 vision:**
  - Library-based Monte Carlo framework
  - Software quality improvements
- **Applications:**
  - Next-generation high performance computers
  - Multi-physics: MCNP often needed within other scientific software
  - Tools to assist users
    - Geometry: Collaborations with industry
      - Allow users to take CAD/CAE, modify and develop mesh-based models; Variance reduction with Sn
    - Radiation Source: ISC – generalized intrinsic source (aged) from any decay library
    - Transport physics: Correlated source/collision physics
    - Tallies: MCNP tools – a package to facilitate user access to MCNP output
      - Users can produce tools to make plots, analyze data, etc without headache of having to parse data
      - One application: radiation detector response

# Thank you!

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